



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:35 AM GMT

PDB ID : 2V0K
Title : CHARACTERIZATION OF SUBSTRATE BINDING AND CATALYSIS OF
THE POTENTIAL ANTIBACTERIAL TARGET N-ACETYLGUCOSAM
INE-1-PHOSPHATEURIDYLTRANSFERASE (GLMU)
Authors : Mochalkin, I.; Lightle, S.; Ohren, J.F.; Chirgadze, N.Y.
Deposited on : 2007-05-14
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

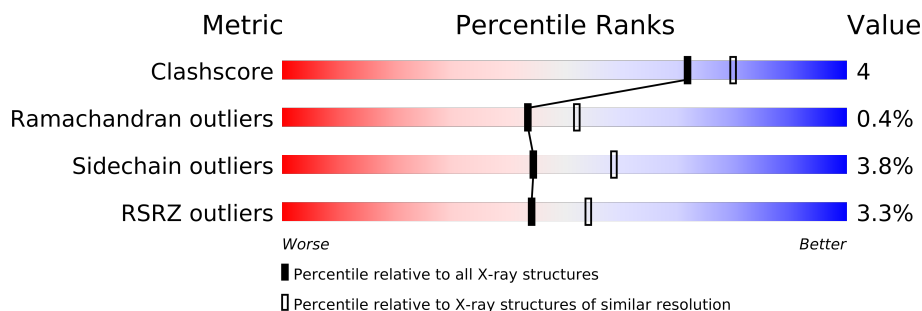
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	456	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	UDP	A	1454	-	X
4	PGE	A	1457	-	X
5	SO4	A	1458	-	X
5	SO4	A	1459	-	X
5	SO4	A	1460	-	X
5	SO4	A	1462	-	X
5	SO4	A	1464	-	X

2 Entry composition i

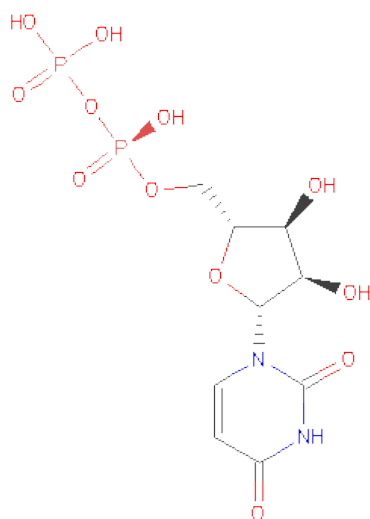
There are 6 unique types of molecules in this entry. The entry contains 3820 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BIFUNCTIONAL PROTEIN GLMU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3423	2147	604	661	11	0	3	0

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



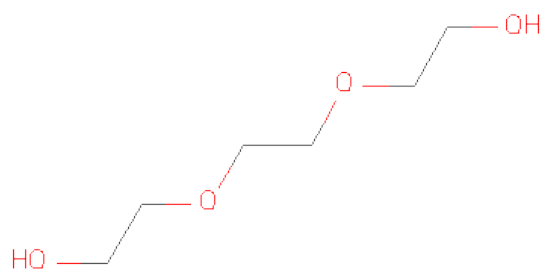
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	25	9	2	12	2	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	304	Total	O	0	0
			304	304		

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- Molecule 1: BIFUNCTIONAL PROTEIN GLMU

I453	LYS	LYS	LYS	LYS	MET
D271	D275	D276	D288	R289	T28
D288	R289	K299	G304	R305	K4
D306	V307	G304	R305	D306	A12
K310	P311	E316	D317	T326	V26
G327	P328	R331	L332	R333	L27
L338	V344	G345	R346	H363	H28
D369	K390	N391	K392	D400	D41
D406	D429	L436	V437	T438	G56
R443	Q443	R444	R451	R452	D60
R453	R454	R455	R456	R457	Q70
R458	R459	R460	R461	R462	A90
R463	R464	R465	R466	R467	P91
R468	R469	R470	R471	R472	D95
R473	R474	R475	R476	R477	N96
R478	R479	R480	R481	R482	E123
R483	R484	R485	R486	R487	D134
R488	R489	R490	R491	R492	R141
R493	R494	R495	R496	R497	E145
R498	R499	R500	R501	R502	N146
R503	R504	R505	R506	R507	G147
R508	R509	R510	R511	R512	N148
R513	R514	R515	R516	R517	V149
R518	R519	R520	R521	R522	Q155
R523	R524	R525	R526	R527	K156
R528	R529	R530	R531	R532	D157
R533	R534	R535	R536	R537	A158
R538	R539	R540	R541	R542	N159
R543	R544	R545	R546	R547	Q162
R548	R549	R550	R551	R552	L163
R553	R554	R555	R556	R557	V187
R558	R559	R560	R561	R562	D200
R563	R564	R565	R566	R567	N209
R568	R569	R570	R571	R572	V212
R573	R574	R575	R576	R577	T218
R578	R579	R580	R581	R582	D219
R583	R584	R585	R586	R587	D256
R588	R589	R590	R591	R592	P259

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	108.66Å 108.66Å 326.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	111.80 – 2.30 19.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (111.80-2.30) 98.6 (19.95-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.23 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.233 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	6 of 62781 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3820	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, PGE, PG4, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	0/3486	0.71	13/4727 (0.3%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	271	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	275	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	400	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	157	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	331	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	256	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	369	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	406	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	200	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	219	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	60	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	95	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3423	0	3458	31	0
2	A	25	0	11	0	0
3	A	13	0	18	0	0
4	A	20	0	28	2	0
5	A	35	0	0	1	0
6	A	304	0	0	5	0
All	All	3820	0	3515	31	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (31) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:444:ARG:HG3	6:A:2288:HOH:O	1.86	0.75
1:A:149:VAL:HB	1:A:212:VAL:HG22	1.74	0.70
1:A:147:GLY:O	6:A:2110:HOH:O	2.15	0.64
1:A:162:GLN:HE22	4:A:1456:PGE:H32	1.64	0.62
1:A:141:ARG:NH1	1:A:155:GLN:OE1	2.36	0.58
1:A:159:ASN:ND2	1:A:162:GLN:H	2.03	0.57
1:A:443:GLN:NE2	6:A:2287:HOH:O	2.37	0.56
1:A:159:ASN:HD22	1:A:159:ASN:C	2.09	0.56
1:A:289:ARG:HD2	1:A:306:ASP:OD2	2.06	0.55
1:A:452:PRO:O	1:A:453:ILE:C	2.46	0.54
1:A:304:GLY:O	1:A:307:VAL:HG13	2.08	0.53
1:A:331:ARG:NH1	6:A:2222:HOH:O	2.40	0.53
1:A:338:LEU:HD21	1:A:344:VAL:HG21	1.94	0.50
1:A:158:ALA:HB3	1:A:163:LEU:HD13	1.93	0.50
1:A:317[B]:ASP:HB3	1:A:334:PRO:HA	1.95	0.47
1:A:436:LEU:HD22	1:A:438:ILE:HG23	1.96	0.47
1:A:259:ARG:NH1	1:A:276:VAL:HG11	2.32	0.45
1:A:28:HIS:HE1	6:A:2014:HOH:O	1.98	0.45
1:A:141:ARG:NH2	1:A:163:LEU:O	2.50	0.45
1:A:70:GLN:HB3	4:A:1457:PGE:H22	1.98	0.44
1:A:12:ALA:HB1	1:A:26:VAL:HG21	2.00	0.44
1:A:451:ARG:O	1:A:453:ILE:N	2.52	0.43
1:A:256:ASP:OD2	1:A:259:ARG:HD3	2.19	0.43
1:A:288:ASP:C	1:A:289:ARG:HG2	2.39	0.43
1:A:326:ILE:HD11	1:A:338:LEU:HD23	2.01	0.42
1:A:310:LYS:HB3	1:A:311:PRO:HD2	2.02	0.42
1:A:333:ARG:HD2	5:A:1460:SO4:O3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:328:PRO:O	1:A:346:ASN:HA	2.20	0.41
1:A:299:LYS:O	1:A:316:GLU:HA	2.20	0.41
1:A:289:ARG:HG3	1:A:306:ASP:OD2	2.21	0.40
1:A:90:ALA:N	1:A:91:PRO:CD	2.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	451/456 (99%)	440 (98%)	9 (2%)	2 (0%)	43 52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	452	PRO
1	A	56	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	368/371 (99%)	353 (96%)	15 (4%)	41 55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	ASP
1	A	156	LYS

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Mol	Chain	Res	Type
1	A	159	ASN
1	A	163	LEU
1	A	187	VAL
1	A	212	VAL
1	A	289	ARG
1	A	317[A]	ASP
1	A	317[B]	ASP
1	A	331	ARG
1	A	346	ASN
1	A	363	HIS
1	A	429	ARG
1	A	436	LEU
1	A	444	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	45	GLN
1	A	57	HIS
1	A	72	ASN
1	A	84	HIS
1	A	96	ASN
1	A	148	ASN
1	A	159	ASN
1	A	211	GLN
1	A	277	ASN
1	A	362	ASN
1	A	408	GLN
1	A	443	GLN
1	A	450	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	UDP	A	1454	-	26,26,26	3.20	5 (19%)	36,40,40	1.42	6 (16%)
3	PG4	A	1455	-	12,12,12	0.45	0	11,11,11	0.30	0
4	PGE	A	1456	-	9,9,9	0.42	0	8,8,8	0.20	0
4	PGE	A	1457	-	9,9,9	0.44	0	8,8,8	0.20	0
5	SO4	A	1458	-	4,4,4	0.20	0	6,6,6	0.11	0
5	SO4	A	1459	-	4,4,4	0.18	0	6,6,6	0.13	0
5	SO4	A	1460	-	4,4,4	0.15	0	6,6,6	0.21	0
5	SO4	A	1461	-	4,4,4	0.19	0	6,6,6	0.23	0
5	SO4	A	1462	-	4,4,4	0.20	0	6,6,6	0.13	0
5	SO4	A	1463	-	4,4,4	0.19	0	6,6,6	0.08	0
5	SO4	A	1464	-	4,4,4	0.14	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDP	A	1454	-	-	0/14/32/32	0/2/2/2
3	PG4	A	1455	-	-	0/10/10/10	0/0/0/0
4	PGE	A	1456	-	-	0/7/7/7	0/0/0/0
4	PGE	A	1457	-	-	0/7/7/7	0/0/0/0
5	SO4	A	1458	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1459	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1460	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1461	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1462	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	1463	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1464	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1454	UDP	PA-O3A	13.48	1.84	1.59
2	A	1454	UDP	PA-O5'	5.44	1.83	1.59
2	A	1454	UDP	PA-O1A	4.33	1.67	1.51
2	A	1454	UDP	C2-N1	3.84	1.42	1.38
2	A	1454	UDP	PA-O2A	2.92	1.68	1.55

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1454	UDP	N3-C2-N1	4.98	120.13	115.97
2	A	1454	UDP	PA-O3A-PB	-2.95	123.02	131.68
2	A	1454	UDP	O5'-C5'-C4'	2.25	117.18	108.94
2	A	1454	UDP	C2-N1-C1'	2.19	119.58	118.21
2	A	1454	UDP	C5-C4-N3	2.08	120.62	116.70
2	A	1454	UDP	O4'-C1'-N1	2.03	112.35	108.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	450/456 (98%)	-0.22	13 (2%) 49 59	12, 24, 41, 54	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	390	ALA	5.7
1	A	146	ASN	5.5
1	A	147	GLY	4.0
1	A	453	ILE	4.0
1	A	134	ASP	3.1
1	A	218	THR	3.0
1	A	96	ASN	2.8
1	A	209	ASN	2.6
1	A	391	ASN	2.5
1	A	123	GLU	2.5
1	A	60	ASP	2.2
1	A	392	LYS	2.2
1	A	145	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	A	1459	5/5	0.29	6.22	71,71,71,71	0
5	SO4	A	1464	5/5	0.34	5.21	60,60,61,61	0
5	SO4	A	1458	5/5	0.27	4.23	62,62,63,63	0
2	UDP	A	1454	25/25	0.28	3.00	59,61,65,65	0
5	SO4	A	1460	5/5	0.22	2.71	54,54,54,54	0
5	SO4	A	1462	5/5	0.34	2.68	81,81,81,81	0
4	PGE	A	1457	10/10	0.18	2.57	45,46,47,48	0
5	SO4	A	1461	5/5	0.18	1.44	65,65,66,66	0
3	PG4	A	1455	13/13	0.12	0.84	32,35,39,41	0
4	PGE	A	1456	10/10	0.14	0.23	41,42,43,44	0
5	SO4	A	1463	5/5	0.14	-0.09	60,60,61,61	0

6.5 Other polymers ⓘ

There are no such residues in this entry.